

Study of Domains in the Ground State of the Two Dimensional Coulomb Glass

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(Dated: October 24, 2016)

We have annealed two dimensional lattice model of Coulomb glass using Monte Carlo simulations to obtain the ground state. We have shown that the energy required to create a domain of linear size L in d dimensions is proportional to L^{d-1} . Using Imry-Ma arguments given for RFIM, one gets $d_c \geq 2$ for Coulomb glass. The investigations in the transition region shows that the domain wall of the metastable state in the charge-ordered phase shifts as disorder is increased to give disordered ground state at higher disorder strength indicating phase coexistence. This coupled with discontinuity in magnetization is an indication of first-order type transition from charge-ordered phase to disordered phase. The structure and nature of Random field fluctuations of the domain in Coulomb glass are inconsistent with the assumptions of Imry and Ma as was also reported for RFIM.

PACS numbers: 71.23.An,75.10.Hk,05.50.+q

The Coulomb glass (CG) is a system in which all electron states are localised and they interact via long-range Coulomb potential. At low temperature, these localised electrons are unable to screen the Coulomb interactions effectively. The long range nature of the Coulomb interactions led to a soft gap [1–3] in the single-particle density of states. This effect changed the conductivity from $\ln \sigma \sim T^{1/4}$ to $T^{1/2}$ as temperature was decreased [4, 5]. Another important effect of Coulomb interaction is correlation effects, i.e. existence of collective hops instead of single electron hops [6]. In recent years, focus has shifted from higher disorder to low disorder region [7]. It has been shown [8] numerically that in three-dimensional (3d) CG, the transition from fluid to the charge-ordered phase (COP) is consistent with the random field Ising Model (RFIM) universality class. Whether the same is true in two-dimensional (2d) CG is yet to be investigated. The motivation of this paper is to understand the importance of Coulomb interactions in domain formation and how the structure of the domain differs from the short range model i.e. RFIM. The Imry-Ma arguments [9] on which the initial theoretical papers on RFIM [10–13] were based, suggested that the energy required for the formation of a domain of linear size L in d -dimensions is $\mathcal{O}(L^{d-1})$. The amount of energy gained from the fluctuations of random field (RF) in the domain is $\mathcal{O}(L^{d/2})$, so the long range order will get destroyed for $d < 2$. The ground state of 3d RFIM shows a transition from ferromagnetic to disordered state as disorder is increased [14]. Binder [15] argued that roughening of domain walls would stabilize the domain in two-dimensions and lead to destruction of ferromagnetic ordering. A rigorous proof was then given by Aizenman and Wehr [16] stating that there is no long-range order in 2d RFIM. These arguments led to a critical dimension $d_c = 2$. Numerical evidence [17, 18] shows roughening of domain walls and the ground state breaking into domains above a length scale

that depends exponentially on the random field strength squared, further strengthened the argument that $d_c = 2$. Contradicting all the above work, evidence of numerical signs of transition in 2d RFIM at $T = 0$ below a critical disorder was shown by Frontera and Vives [19]. In a seminar [20] in 2012, Aizenman also claims that the 2d RFIM exhibits a phase transition. In 2013 Sinha and Mandal [21] used Monte Carlo simulations to show that for weak fields 2D RFIM possesses long-range ordering. The validity of the Imry-Ma arguments was tested by doing numerical calculations. The properties of domains were significantly different from the assumptions made by Imry and Ma [22, 23].

In this letter, we investigate the possibility of transition from charge-ordered phase (COP) to disordered phase (DP) and the properties of domain structure in the ground state via Monte Carlo (MC) annealing of the two-dimensional (2d) CG lattice model with on-site disorder [24, 25]. Our results are as follows: (i) We found indication of a first-order type transition from COP to DP as seen in 2d RFIM [18]. (ii) Although the long-range interactions in the system remain unscreened, the interaction energy of the domain is still $\mathcal{O}(L^{d-1})$ which allows one to use the Imry-Ma argument. (iii) The domain wall of the metastable state in the COP at (W_c^-) shifts to give disordered ground state at (W_c^+) . (iv) In the disordered phase (W_c^+) , our results shows that the domain structure and the nature of random-field (RF) fluctuations in the domain contradict the Imry-Ma assumptions but are consistent with the numerical work on RFIM [22].

We consider the classical 2d CG lattice model, in which the electron states are assumed to be localized around the sites of a regular lattice with lattice spacing $a \equiv 1$. We work with a case of half filling which implies that the number of electrons are half the total number of sites (N). We use the pseudospin variables $S_i = n_i - 1/2$ where $n_i \in 0, 1$ is the occupation number at site i . The Hamil-

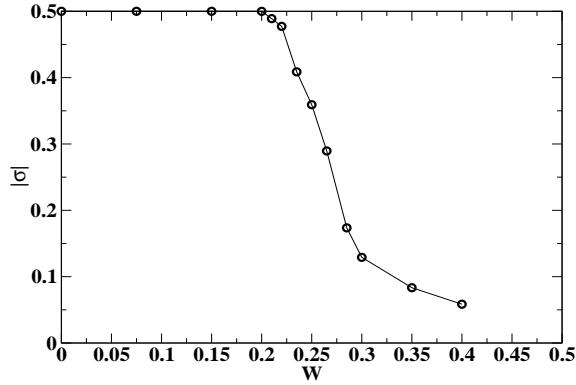


FIG. 1. (Color online) Staggered magnetisation (σ) at different disorder (W).

tonian of the system can now be written in spin language as

$$H = \sum_i \phi_i S_i + \frac{1}{2} \sum_{i \neq j} J_{ij} S_i S_j \quad (1)$$

where the unscreened Coulomb interactions are described as $J_{ij} = e^2/\kappa R_{ij}$, κ is the dielectric constant and R_{ij} is the distance between site i and j . We are using periodic boundary condition (PBC). ϕ_i 's denote the random on-site energies, chosen randomly from a box distribution with interval $[-W/2, W/2]$. The particle-hole symmetry with symmetric disorder distribution lead to $\mu = 0$. All the energies were measured in the unit of $e^2/\kappa a$.

We are here proposing an argument to calculate the energy of a regular domain (which is square for $d = 2$ and cube for $d=3$) created in the ground state of a d -dimensional CG lattice model at half filling. The Hamiltonian of the system in terms of Hartree energy (ε_i) can be written as $H = \frac{1}{2} \sum_{i=1}^N (\varepsilon_i + 2\phi_i) S_i$ where $\varepsilon_i = \sum_{j \neq i} J_{ij} S_j$. In the zero disorder limit, the ground state of a CG system has Antiferromagnetic ordering. So Hartree energy at each site is equal to d -dimension Madelung energy (ε_d). Staggered magnetisation defined as $\sigma = 1/N \sum_{i=1}^N \sigma_i$, is the order parameter where $\sigma_i = (-1)^i S_i$. Cluster of nearest -neighbour sites which have same σ_i is defined as a domain. As the system has anti-ferromagnetic ordering, each row on the lattice is charge neutral. For any charge, the contribution to its Hartree energy can be divided into two parts (a) from charges on the line (plane) on which the site is located (b) charges on few rows (planes) just above and below the charge under consideration and negligible contribution coming from rest of the lines(planes) [26]. There is no surface effect as we are using PBC. Now if we consider a large regular domain then the Hartree energy of the sites inside the domain will be equal to ε_d using the reasoning given above. Extending the same argument, the Hartree energy of the site on the domain wall becomes approximately equal to $d - 1$ Madelung

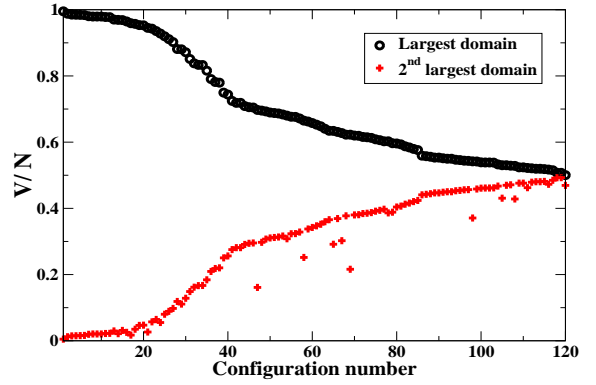


FIG. 2. (Color online) Largest (\circ) and second largest ($+$) domain size (V) in the DP (W_c^+) divided by the system size N . The largest domains are sorted in descending order.

energy (ε_{d-1}). This is because, for a site i on the domain wall, $\varepsilon_i = \sum J_{ij}^F \sigma_j^{out} + \sum J_{ij}^F \sigma_j^{in} + \sum J_{ij}^F \sigma_j^{wall}$ where $J_{ij}^F = J_{ij}(-1)^{i+j}$ and $\sigma_j^{out}, \sigma_j^{in}, \sigma_j^{wall}$ describes σ of sites outside the domain wall, inside the domain wall and on the domain wall respectively. The first two terms in the summation cancels out because $\sigma_j^{in} = -\sigma_j^{out}$. The third term is $\sim \varepsilon_{d-1}$ for a large domain. So the energy required to create a domain wall is $1/2(\varepsilon_d - \varepsilon_{d-1}) \times P$ where P is proportional to L^{d-1} . Since energy gained from RF is still $\mathcal{O}(L^{d/2})$, Imry-Ma argument can be applied to a regular domain. This explains why 3d CG is in the same universality class of RFIM as claimed earlier [8]. Whether long range order can exist for 2d CG is now a matter of further investigations.

We have done simulated annealing using Monte Carlo (MC) technique for 64×64 system. The initial system was completely random spin configuration $\{S_i\}$ with half sites assigned with $S_i = 1/2$ and the other half with $S_i = -1/2$. Annealing using Metropolis algorithm [27] was done from $T = 1$ to $T = 0.01$. Our longest run was 5×10^5 MCS per site at $T = 0.01$. The investigations were carried out for different disorders strengths ($W = 0.0$ to 0.40) using two different approaches. (a) For each W , uncorrelated $\{\phi_i\}$ were used. (b) In the second approach, the sign of $\{\phi_i\}$ at each site were fixed and the strength of the randomness (W) was increased [17, 23]. The second approach has an advantage that one is able to see the evolution of the metastable state of COP to the ground state of DP as W is increased. After annealing was completed, we found system consisted of mostly two large domains and few small domains. The domains were identified using Hoshen-Kopelman algorithm [29]. We then calculated the domain-domain interactions and found it to be negligible. This allowed us to flip the domains one by one to get the minimum energy state (ground state). We do not claim that our method finds the exact ground state.

Using the first approach, the behaviour of σ at different

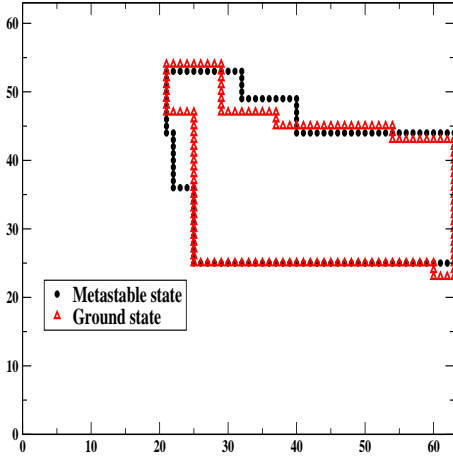


FIG. 3. (Color online) Domain wall of Metastable state at $W = 0.235$ and domain wall of ground state at $W = 0.25$ are plotted for one of the configurations.

disorder strengths (W) is shown in FIG. 1. $|\sigma|$ changes from 0.5 to 0, indicating a transition from COP to DP. Further investigations in this paper were done using the second approach where we solely focus on ground state at W_c^+ and the metastable state of the COP at W_c^- (for each disorder configuration W_c will be different). FIG 2 shows the size of the largest and second largest domains (which is non-zero for all configurations) in the ground state. For most of the configuration COP breaks into two large domains as we move from W_c^- (where $\sigma = \pm 0.5$) to W_c^+ (where $\sigma \approx 0.0$) which results into discontinuity in staggered magnetisation at each configuration of disorder. So in the transition region the two phases coexist, which is a characteristic feature of a first-order transition. In simulations of 3d RFIM at finite T [30] and $T = 0$ [14] small value of magnetization exponent indicative of discontinuity in magnetization at the transition was found but other parameters rule out the possibility of a first order transition. To further prove coexistence, we then compared the domains formed in the ground state at W_c^+ with the domains of the metastable state at W_c^- . From FIG 3, one can see that the domain wall of the metastable state shifts to give the ground state as W was increased slightly. This shows that free energy which is equal to energy at $T = 0$ has two minimas centred at $|\sigma| = 0.5$ and $|\sigma| \approx 0.0$, indicative of first order transition. From FIG. 2, one can see that in first few configurations, size of the second largest cluster is very small. One such configuration is shown in FIG. 4, where the domains similar to the metastable state reappears as W is increased further. As far as the phase transition is concerned, the discontinuous change in σ is preserved.

To test the validity of the Imry-Ma arguments on CG model, we focussed on the structure and the nature of RF fluctuations of the domains in the ground state. The compactness of the domains was checked by using a the power law relation [22] $S \approx V^\tau$, where the surface (S)

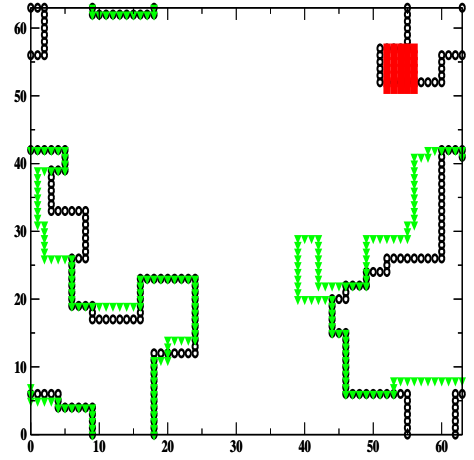


FIG. 4. (Color online) Domain Wall of metastable state (\circ) at $W = 0.22$, ground state (\blacksquare) at $W = 0.235$ and ground state (∇) at $W = 0.25$.

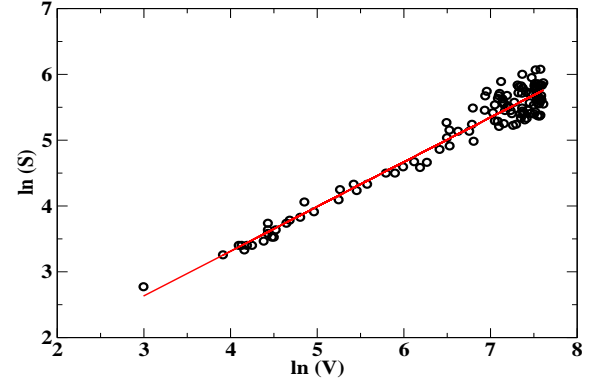


FIG. 5. (Color online) Logarithmic plot of surface vs size for the determination of surface exponent τ for 2d CG.

of the domain denote the number of sites on the domain wall and the volume (V) of the domain is the total number of sites in the domain. The value of the surface exponent τ for a compact domain is $1 - 1/d$. FIG 5 proves the validity of the relation for the CG system and the value of the surface exponent is $\tau = 0.6756$. The high value of τ indicates that the domains are non-compact. Our theoretical argument for $DE \propto P$ can be easily extended to a compact domains but needs to be numerically tested for non-compact domains. The plot of DE vs P (FIG. 6) shows that the relation $DE = \eta \times P$ (where $\eta = 0.0335$) is valid. The value of η calculated numerically is slightly higher than the predicted theoretical value for 2d which is $\eta = 1/2(\epsilon_{2d} - \epsilon_{1d}) \approx 0.0285$. To understand this agreement in η values, we have plotted the distribution of Hartree energies of the sites on the domain wall (ϵ_i^{wall}) and inside the domain wall (ϵ_i^{inside}) in FIG. 7. The Hartree energies of the sites on the wall and inside the wall are distributed symmetrically around

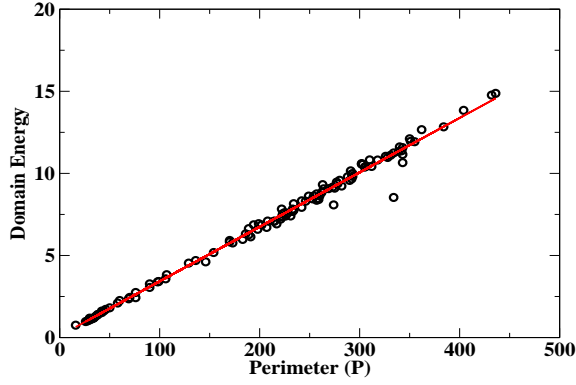


FIG. 6. (Color online) The domain energy vs perimeter of the domain.

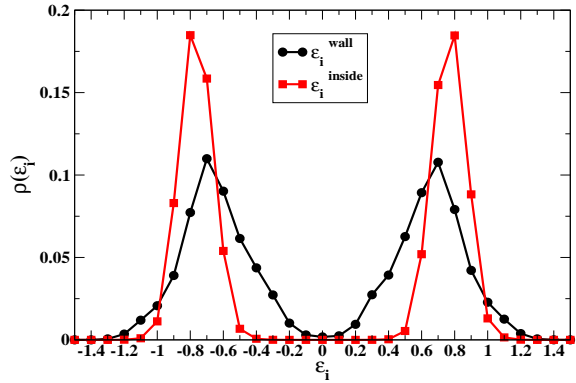


FIG. 7. (Color online) Distribution of Hartree energy of the sites on the domain wall (ε_i^{wall}) and on sites inside the domain wall where domain wall sites are excluded (ε_i^{inside}).

ε_{1d} and ε_{2d} respectively. This is the reason why our numerical results matches our argument given for DE calculation. Next we tested the hypothesis that the total random-field fluctuations (F) in a domain is typically a rms deviation and is proportional to the square root of V . A general power law expression [22] can be written as $F \approx V^\lambda$ where λ was considered as an undetermined exponent. This relation is verified from FIG. 8(Top) and the corresponding value of $\lambda = 0.6415$. This value of λ is significantly higher than the theoretical value ($\lambda = 1/2$) assumed in RFIM. We have also calculated the ratio F_{wall}/F . In FIG 8(center) one can see that the range of the ratio is 40% to 60% for most of the configurations, indicating that the random field energy of the domain is contained more in the domain boundary. We then calculated the random-field fluctuation of the sites on the domain wall (F_{wall}) and of the sites which are just outside the domain wall (F_{out}). FIG. 8(bottom) shows that the random-field fluctuations are proportional to the perimeter of the domain and not its square root as assumed in previous theories. We have also checked that the location of the domains is independent of the initial spin configuration chosen and is determined by the random-field

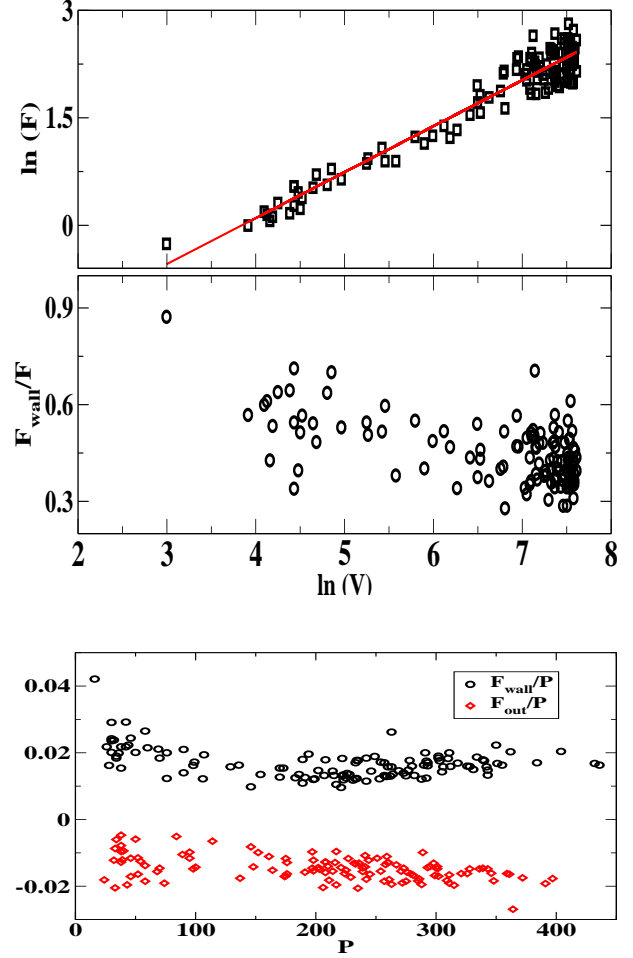


FIG. 8. (Color online). Top: Logarithmic plot of RF fluctuation(F) vs volume(v) of the domains in ground state. The power law relation $F \approx V^\lambda$ holds, giving $\lambda = 0.6415$. Center: RF fluctuation at domain wall(F_{wall}) and layer just outside the domain wall (F_{out}). The y coordinate is the ratio F/P , with P the perimeter length, and the x ordinate is the perimeter length P . Bottom: Ratio F_{wall}/F_{fluc} , where F_{fluc} is the total RF fluctuation in the domain at ground state.

configurations. The strong RF fluctuations on the wall lead to the pinning of the domain wall which is the reason for the metastability of the domains. So our results suggests that the domains in the ground state are pinned, non-compact and the RF fluctuations are contained more at the domain boundary. These results are consistent with the numerical work [22, 23] done on RFIM.

Conclusions- We have shown that the Imry-Ma argument for short range RFIM can be extended to CG system at half filling leading to $d_c = 2$. To verify the argument, we numerically investigated the 2d CG lattice model using MC annealing. Our numerical work shows a phase transition from COP to disordered phase of first-order type. The transition is driven by the rearrangement of domain wall of the metastable state in COP as W is

increased to give disordered phase. We are not claiming that our result is a proof of a thermodynamic transition. The domains formed are non-compact and the RF fluctuations are contained more at the domain wall, in contradiction with Imry-Ma assumptions.

We wish to thank NMEICT cloud service provided by BAADAL team, cloud computing platform, IIT Delhi for the computational facility. Preeti Bhandari acknowledges UGC, Govt. of India for financial support through UGC-BSR fellowship (F.25-1/2013-14(BSR)/7-93/2007(BSR)).

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